IN THE CLAIMS

This is a complete and current listing of the claims, marked with status identifiers in parentheses. The following listing of claims will replace all prior versions and listings of claims in the application.

1. (Currently Amended) A ~~Method~~ method for sampling a state space by iteratively generating states $x_{i,t}$ and their weighting factors $\tilde{\rho}_{i,t}$, wherein the index i is the iteration parameter and the index t distinguishes different states $x_{i,t}$ generated by an iteration i, the method ~~is consisting of~~ comprising:

a first step for selecting an initial sampling distribution function $\rho_1(x)$,

a fifth step for performing an analysis

and an iteration procedure including

a second step for generating N_j states $x_{j,t}$ by a numerical sampling algorithm and

a fourth step for testing at least one criterion to decide whether to continue the iteration procedure or to stop the iteration procedure and to go to a fifth step in order to perform the analysis using the simulated data, wherein

~~characterized in that~~ the iteration procedure further includes

a third step determining weighting factors $\tilde{\rho}_{i,t}$ for states $x_{i,t}$ generated so far by using sampling distribution functions $\rho_i(x)$ determined so far and

a fitting step for determining a sampling distribution function $\rho_j(x)$ for the next iteration by fitting $\rho_j(x)$ to $\tilde{\rho}_{i,t}O(x_{i,t})$ for states $x_{i,t}$ generated so far, wherein $O(x_{i,t})$ is a function, respectively a property, of the states $x_{i,t}$.

2. (Currently Amended) Method as claimed in claim 1, wherein the sampling distribution function $\rho_j(x)$ of at least one iteration is fitted such that it ~~maximises~~ maximizes an objective

function preferably defined as a function of local comparisons between the sampling

distribution function and the product $\tilde{p}_{i,t}O(x_{i,t})$.

3.   (Currently Amended)   Method as claimed in claim 1 ~~or 2~~, wherein the sampling distribution

function $\rho_j(x)$ of at least one iteration is fitted such that the sampling distribution function

$\rho_j(x)$ is large for at least one state $x_{i,t}$ with a large product $\tilde{p}_{i,t}O(x_{i,t})$, and tends to be small

for states with a small product $\tilde{p}_{i,t}O(x_{i,t})$.

4.   (Currently Amended)   Method as claimed in ~~one of claims~~ claim 1 ~~to~~ 3, wherein the

sampling distribution function $\rho_j(x)$ of at least one iteration is a function with at least one

constraint.

~~, preferably having an extreme value in the region of at least one selected state $x_{j,constr}$ and having~~

~~vanishing values at a distance from the at least one selected state $x_{j,constr}$, wherein the~~

~~constraint is preferably a harmonic constraint with at least one constant k_{constr} defining the~~

~~strength of the constraint at the selected state $x_{j,constr}$.~~

5.   (Currently Amended)   Method as claimed in claim 4, wherein the sampling distribution

function $\rho_j(x)$ of at least one iteration is the distribution function of the system with

constraints or a multicanonical distribution function with constraints.

6.   (Currently Amended)   Method as claimed in claim 1 ~~or 2~~, wherein the numerical sampling

algorithm of at least one iteration generates correlated states $x_{j,t}$ ~~, wherein the sampling~~

~~distribution function $\rho_j(x)$ preferably has a maximum that biases sampling into a sub-region~~

~~of the state space, wherein the sampling distribution function $\rho_j(x)$ is preferably fitted such~~

~~that the maximum is in a region where the product $\tilde{p}_{i,t}O(x_{i,t})$ has a maximum, and wherein~~

~~the sampling preferably starts from a state close to the maximum of the sampling distribution~~

~~function $\rho_j(x)$~~.

7.   (Currently Amended)   Method as~~.~~ claimed in ~~one of~~ claims 4 ~~to 6~~, wherein the fitting of

$\rho_j(x)$ is done by selecting states $x_{i,t}$ for which the product $\tilde{\rho}_{i,t}O(x_{i,t})$ has extreme values and

by using the selected states $x_{i,t}$ to define the region in which $\rho_j(x)$ has extreme values.

8.   (Currently Amended)   Method as claimed in ~~one of~~ claims 1 ~~to 6~~, wherein parameters of the

sampling distribution function $\rho_j(x)$ of at least one iteration are determined by a linear least

square fit of the logarithm of the un-normalized sampling distribution function $\rho_j(x)$ to the

logarithm of the product $\tilde{\rho}_{i,t}O(x_{i,t})$.

9.   (Currently Amended)   Method as claimed in ~~one of~~ claims 1 ~~to 8~~, wherein the normalization

constant of the sampling distribution function $\rho_j(x)$ of at least one iteration is estimated from

the sampled states $x_{i,t}$ and their weighting factors $\tilde{\rho}_{i,t}$.

10.   (Currently Amended)   Method as claimed in ~~one of~~ claims 1 ~~to 9~~, wherein at least three

iterations are done.

11.   (Currently Amended)   Method as claimed in ~~one of~~ claims 1 ~~to 10~~, wherein the function

$O(x)$ is a function of a set of at least two functions $\Theta=\{O_1(x),O_2(x),...,O_{N_{prop}}(x)\}$, ~~preferably~~

~~including at least one of the following functions~~

~~at least one property for which at least one estimate is derived in the analysis of the fifth step,~~

~~at least one function that is large for states that must be sampled to ensure transitions between~~

~~important regions,~~

~~the inverse of the probability distribution function of at least one property of the system, and~~

~~the inverse of the probability distribution of the negative logarithm of the distribution function~~

~~of the system~~.

12.   (Currently Amended)   A computer software product for sampling a state space by iteratively

generating states $x_{i,t}$ and their weighting factors $\tilde{p}_{i,t}$, wherein the index i is the iteration

parameter and the index t distinguishes different states $x_{i,t}$ generated by an iteration i, said

product ~~is characterized by~~including a computer-readable medium in which program

instructions are stored, which instructions, when read by a computer, enable the computer to:

select an initial sampling distribution function $\rho_1(x)$,

to execute a fifth step for performing an analysis,

and to execute an iteration procedure including,

a second step for generating N_j states $x_{j,t}$ by a numerical sampling algorithm and

a fourth step for testing at least one criterion to decide whether to continue the iteration

procedure or to stop the iteration procedure and to go to a fifth step in order to perform the

analysis using the simulated data, wherein

~~characterized in that~~the iteration further includes

a third step determining weighting factors $\tilde{p}_{i,t}$ for states $x_{i,t}$ generated so far by using

sampling distribution functions $\rho_i(x)$ determined so far and

a fitting step for determining a sampling distribution function $\rho_j(x)$ for the next iteration by

fitting $\rho_j(x)$ to $\tilde{p}_{i,t}O(x_{i,t})$ for states $x_{i,t}$ generated so far, wherein $O(x_{i,t})$ is a function,

respectively a property, of the states $x_{i,t}$.

13.   (New)   Method as claimed in claim 2, wherein the sampling distribution function $\rho_j(x)$ of at

least one iteration is fitted such that the sampling distribution function $\rho_j(x)$ is large for at

least one state $x_{i,t}$ with a large product $\tilde{p}_{i,t}O(x_{i,t})$, and tends to be small for states with a

small product $\tilde{p}_{i,t}O(x_{i,t})$.

14.   (New)   Method as claimed in claim 1, wherein the sampling distribution function $\rho_j(x)$ of at

least one iteration is a function with at least one constraint, having an extreme value in the region of at least one selected state $x_{j,constr}$ and having vanishing values at a distance from the at least one selected state $x_{j,constr}^{\bullet}$.

15. (New) Method as claimed in claim 1, wherein the sampling distribution function $\rho_j(x)$ of at least one iteration is a function with at least one constraint, having an extreme value in the region of at least one selected state $x_{j,constr}$ and having vanishing values at a distance from the at least one selected state $x_{j,constr}$, wherein the constraint is a harmonic constraint with at least one constant k_{constr} defining the strength of the constraint at the selected state $x_{j,constr}$.

16. (New) Method as claimed in claim 1, wherein the numerical sampling algorithm of at least one iteration generates correlated states $x_{j,t}$, wherein the sampling distribution function $\rho_j(x)$ has a maximum that biases sampling into a sub-region of the state space, wherein the sampling distribution function $\rho_j(x)$ is fitted such that the maximum is in a region where the product $\tilde{\rho}_{i,t} O(x_{i,t})$ has a maximum, and wherein the sampling starts from a state close to the maximum of the sampling distribution function $\rho_j(x)$.

17. (New) Method as claimed in claim 1, wherein the function $O(x)$ is a function of a set of at least two functions $\Theta = \{O_1(x), O_2(x), ..., O_{N_{prop}}(x)\}$, including at least one of the following functions:
at least one property for which at least one estimate is derived in the analysis of the fifth step,
at least one function that is large for states that must be sampled to ensure transitions between important regions,
the inverse of the probability distribution function of at least one property of the system, and
the inverse of the probability distribution of the negative logarithm of the distribution function of the system.

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18. (New) A computer-readable medium comprising executable program instructions configured to cause a computer to perform the method of claim 1.

19. (New) A computer program, adapted to cause a computer to perform the method of claim 1.

20. (New) A computer-readable medium comprising the computer program of claim 19.